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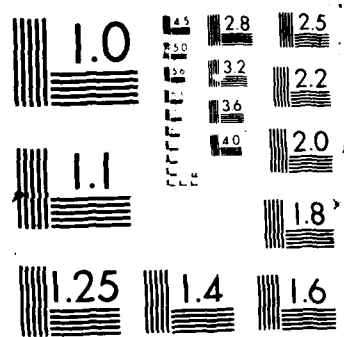
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ORDERING METHODS FOR SPARSE MATRICES AND VECTOR COMPUTERS

AFOSR Contract F49620-85-C-0057

Report No. 2 **AFOSR-TR. 87-0967**

Final Report

by

Horst D. Simon

Boeing Computer Services Company

August 15, 1986

KEY WORDS AND PHRASES: Linear equations, sparse matrices, reordering algorithms, Choleski factorization, Gauss elimination, frontal methods, multifrontal methods, minimum degree ordering, quotient tree algorithm, vector computers, parallel computers.

ABSTRACT: This report summarizes the activities at Boeing Computer Services Company on AFOSR Contract F49620-85-C-0057 from April 16, 1985 until August 15, 1986. Five tasks are defined in our analysis of quotient tree algorithms and frontal methods: analyses of multi-frontal methods, creation of symmetric out-of-core minimal storage sparse elimination schemes, analyses of quotient tree orderings, and completion of the Harwell-Boeing sparse matrix test collection. Reports on the progress of the work on the five tasks are given, relevant reports and publications of project personnel are listed and related sparse matrix activities are discussed.



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INTRODUCTION

The solution of systems of large sparse linear equations is a fundamental computational step in the numerical solution of many scientific and engineering problems. A key aspect of the solution is the choice of a reordering heuristic, in which the equations are presented in a new order that reduces some measure of the cost of the solution. Algorithms for obtaining the optimal reordering are usually too expensive, therefore for all practical purposes only reordering heuristics are considered, which produce a near optimal reordering. Different reordering heuristics have arisen in many disciplines, reflecting different types of sparse matrix systems and different approaches to cost.

This research project was concerned with improving our understanding of several different classes of reordering heuristics. One is the general category of frontal methods, a second category are quotient tree orderings. All these heuristic algorithms are in some sense general purpose, but have been developed for different problems and with different goals in mind. Our general objectives were to understand the relationship of frontal methods to general sparse methods, and to characterize and evaluate quotient tree methods. This report describes the current status of the project. The following topics are covered by this report: research objectives, status of the research effort, relevant publications by the project personnel, professional personnel associated with the research effort, and related sparse matrix activities at Boeing Computer Services.

RESEARCH OBJECTIVES

The research objectives were broken down into five tasks. The tasks, as described in Report No. 1 from April 10, 1986, were:

Task 1: Analysis of Multi-Frontal Orderings.

This task includes an analysis of the storage requirements for frontal factorizations of symmetric indefinite matrices and an investigation of methods combining both the advantages of frontal and standard elimination schemes. Our plan for this analysis consisted of the following subtasks:

- (a) formalization of proofs of equivalence
- (b) analysis of space requirements
- (c) empirical study of the behavior for large positive definite systems
- (d) empirical evaluation of the behavior for large indefinite systems
- (e) preparation of a technical paper containing the results of a) - d)
- (f) possible modifications to multi-frontal techniques based on the earlier subtasks.

Task 2: Creation of a Symmetric Indefinite Out-of-Core General Sparse Solver.

This activity is an attempt to exploit Liu's work on out-of-core solution of positive definite linear systems to produce a generalization for symmetric indefinite systems. The approach is to use Liu's experimental code as a prototype, to be modified into a code that approaches the indefinite case in a generalization of the manner used in the multifrontal codes. Our expectation is that the behavior of the new code will mirror that of the multifrontal code, which will confirm the explanation of the relationships between them.

The plan for this work was as follows:

- (a) conversion of Liu's code from York to Boeing Cray
- (b) removal of compression from the subscript data structure
- (c) incorporation of 2 by 2 pivoting for indefiniteness
- (d) empirical evaluation of the indefinite code on test problems derived from large structural eigenvalue problems
- (e) preparation of a technical paper on the results

Task 3: Analysis of an Out-of-Core General Sparse Algorithm.

One of the key differences between multifrontal and current general sparse algorithms is the ordering of operations performed in Gaussian elimination. General sparse formulations use a GAXPYI or inner product formulation, whereas frontal codes use a SAXPY or outer product formulation. Another outer product formulation using SAXPYI's (indexed SAXPY's) is possible and is quite similar in spirit to the so-called minimum storage sparse elimination algorithm. We proposed to investigate possible out-of-core outer product factorization according to the following subtasks:

- (a) modify symbolic factorization from (2b) to predict storage requirements for the new algorithm
- (b) use the experimental code from 2 as the basis for creating a code to use in testing the numerical behavior of the new algorithm
- (c) evaluate the new code on the standard large test problems
- (d) prepare technical paper on the results.

Task 4: Analysis of Quotient Tree Orderings.

The evaluation of the refined quotient tree ordering (RQT) by George and Liu on some large three dimensional structural analysis problems has shown this method to be very efficient, in particular with respect to storage requirements. Recently Zmijewski and Gilbert have published a theoretical analysis of alternative quotient tree algorithm for certain model problems. The objectives of this task were to analyze these and other quotient tree algorithms and investigate a possible general characterization of quotient tree algorithms, with the possibility of generating new ordering heuristics. The planned subtasks were:

- (a) characterize relationship of level structures and quotient tree orderings
- (b) preliminary empirical study of quotient tree orderings

- (c) evaluate hole breaking strategies on model problem
- (d) evaluate other modifications to quotient tree orderings on model problems
- (e) empirical study using modified SPARSPAK code addressing results of (c) and (d)
- (f) evaluate tree structure as basis for parallel implementation
- (g) investigate relationship of out-of-core quotient tree factorization algorithm to multifrontal and general sparse work
- (h) prepare technical paper

Task 5: Completion and Publication of the Harwell-Boeing Sparse Matrix Test Collection.

The Harwell-Boeing test matrix collection has been a useful tool for numerous researchers. In particular, examples of very large realistic problems have been very important in evaluating the real performance of proposed algorithms. A more flexible updating and distribution system was needed for making the collection available to other researchers and in preparing a formal publication on the collection. A number of very large structural engineering examples from Boeing was planned to be added to the collection. Dr. Iain Duff from AERE Harwell is a collaborator on this task. The subtasks were:

- (a) finalizing current collection
- (b) completion of distribution system
- (c) preparation of formal announcement (paper).

STATUS OF THE RESEARCH EFFORT

Significant progress was made in all of the five tasks, and Task 5 was essentially completed. We anticipate to complete Tasks 1 - 4 in the option year of the contract. The progress made so far is described in detail below:

Task 1. Tasks 1(a) through 1(d) have been completed during the first year of the project. The relationship between multifrontal and general sparse algorithms have been formalized. We have been able to show that given the same ordering, the number of operations performed by a multifrontal implementation of Gaussian elimination is equivalent to the number of operations in a general sparse scheme. The in-core storage requirements for general sparse elimination, frontal method, multifrontal method have been analyzed and compared on a variety of problems and with a number of different orderings. The orderings considered were reverse Cuthill-McKee, automated nested dissection, quotient minimum degree, multiple minimum degree, the MA27 minimum degree ordering, and the ordering generated by Liu's out-of-core solver. Our preliminary findings indicate that the multifrontal scheme required least in-core storage among the methods considered.

Task 2. Tasks 2(a) through 2(c) have been completed. A prototype sparse symmetric indefinite out-of-core solver has been implemented. The implementation is based on Liu's out-of-core solver which has been converted

to the Boeing CRAY. This symmetric positive definite solver has been modified to incorporate two by two pivoting for the symmetric indefinite case. Columns of the matrix, which cannot be eliminated for stability reasons as indicated by the Bunch-Kaufmann test, are put on a stack. Implementing the stack and accounting for the additional fill-in caused by the interchanges required some major recoding. In the current version of the code some details in the garbage collection on the stack require further refinement. After these modifications have been implemented, we will be able to evaluate the code on large indefinite structures problems, and compare its performance to the multifrontal method.

Task 3. Tasks 3(a) through 3(c) have been completed. Three variants of a new class methods called tree profile methods have been implemented. The tree profile methods are frontal methods based on the elimination tree. In version 1 a complete path from a the leaf to be eliminated to the root is kept in core. Version 2 only keeps in core the complete path from the leaf to the highest ancestor directly connected to the leaf. The third version finally only has in core directly connected ancestors of a leaf node. The third version obviously requires the minimum amount of in-core storage. Its implementation is not much more complicated than the implementations of versions 1 and 2. Thus among tree profile methods, version three appears to be most efficient.

Tree profile methods are based on a dense SAXPY or outer product formulation. They were compared to a forward sparse storage scheme using indexed SAXPY's (SAXPYI's). The forward sparse scheme is closely related to the minimum storage Gaussian elimination scheme by Sherman. In numerical tests these methods were evaluated in a similar setup as in Task 1, which allows a direct comparison to multifrontal and general sparse methods. It turns out that tree profile methods require somewhat more storage and increased operation count than forward sparse methods. However, the advantage of tree profile methods is to perform dense SAXPY's instead of sparse SAXPYI's. Hence tree profile methods have a longer average vector length.

Task 4. Tasks 4(a), (b), (d), and (e) have been completed. We have been able to relate quotient tree orderings directly to elimination trees, and thus developed a way to generate quotient tree partitioning from arbitrary sparse matrix orderings. Based on a theoretical analysis on regular grid problems, quotient tree orderings derived from a minimum degree ordering appeared to be promising, and have been implemented. The variants which have been implemented include a level structure rooted at the node ordered last by the minimum degree ordering. This ordering generated generally wide quotient trees, which will be of use in the parallel implementation of RQT to be studied in the future. Overall our empirical studies indicate that none of the new RQT orderings considered significantly improved over SPARSPAK RQT with regards to storage and/or operation counts. However, if the results also showed that RQT's performance is comparable to and sometimes better than minimum degree on large structured problems.

Task 5. Task 5 has been completed. During the project year several new matrices have been added to the collection, which now contains about 225 matrices. Some very large matrices have been obtained from structural analysis models ranging up to 44,609 unknowns. The collection has been extended to include complex matrices, and right hand sides for iterative problems. The matrices now can be accessed through a data base, which allows a user to extract only matrices of a certain problem class (e.g. chemical engineering) or matrix type (e.g. symmetric). The availability of the collection to the general scientific community will be announced in a paper, which is currently under preparation by Iain Duff at AERE Harwell.

RECENT RELEVANT REPORTS AND PUBLICATIONS OF THE PROJECT PERSONNEL

C. Ashcraft, "Parallel Reduction Methods for the Solution of Banded Systems of Equations", General Motors Research Laboratories Publication GMR-5094, 1985, (submitted for publication).

C. Ashcraft, "A Moving Computation Front Approach to Vectorizing ICCG Calculations", General Motors Research Laboratories Publication GMR-5174, 1985, (submitted for publication).

C. Ashcraft, G. M. Shook, and J.D. Jones, "A Computational Survey of Conjugate Gradient Preconditioners on the Cray 1-S", General Motors Research Publication GMR-5229, 1986, (submitted for publication).

A.M. Erisman, R.G. Grimes, J.G. Lewis, W.G. Poole, Jr., and H.D. Simon, "Evaluation of Orderings for Unsymmetric Sparse Matrices" (to appear SIAM J. Sci. Stat. Comp. 1986).

D.S. Dodson and J.G. Lewis, "Issues Relating to Extension of the Basic Linear Algebra Subprograms," SIGNUM Newsletter, Vol. 20, No. 1, January 1985, pp. 19-22.

D.S. Dodson and J.G. Lewis, "Proposed Sparse Extensions to the Basic Linear Subprograms," SIGNUM Newsletter, Vol. 20, No. 1, January 1985, pp. 22-25.

R.G. Grimes, J.G. Lewis, L. Komzsik, D.Scott, and H.D. Simon, "Shifted Block Lanczos Algorithm in MSC/NASTRAN", Proceedings of the MSC/NASTRAN User's Conference, Los Angeles, March 1985.

R.G. Grimes, J.G. Lewis, and H.D. Simon, "Eigenvalue Problems and Algorithms in Structural Engineering" to appear in the Proceedings of the IBM Europe Workshop on Eigenvalue Problems, edited by J. Cullum and R. Willoughby, North-Holland, 1986.

R.G. Grimes, J.G. Lewis, and H.D. Simon, "A Block Shifted Lanczos Algorithm for Eigenvalue Problems in Structural Engineering", Report ETA-TR-39, Boeing Computer Services, 1986.

R.G. Grimes, H. Krakauer, J.G. Lewis, H.D. Simon, and S.-H. Wei, "The Solution

of Large Dense Generalized Eigenvalue Problems on the Cray X-MP/24 with SSD", (to appear J. Comp. Physics).

J.G. Lewis and H.D. Simon, "The Impact of Hardware Gather/Scatter on Sparse Gaussian Elimination", Report ETA-TR-33, Boeing Computer Services, June 1986 (submitted to SIAM J. Scient. Stat. Computing).

H. D. Simon, Incomplete LU Preconditioners for Conjugate-Gradient-Type Iterative Methods, Proceedings of the Eighth SPE Symposium on Reservoir Simulation, Dallas, Texas, February 1985.

RECENT PRESENTATIONS AT PROFESSIONAL MEETINGS

C. Ashcraft, "The Solution of Banded Systems of Equations in Block-Tridiagonal Form Using Odd-Even Reduction", Second SIAM Conference on Applied Linear Algebra, Raleigh, N.C., 1985.

C. Ashcraft, "A Computational Survey of Conjugate Gradient Preconditioners", SIAM National Meeting, Boston, July 1986.

R.G. Grimes, L. Komzsik, J.G. Lewis, D.S. Scott and H.D. Simon, "Shifted Block Lanczos Algorithm in MSC/NASTRAN," MSC/NASTRAN User's Conference, Los Angeles, California, March 1985.

R.G. Grimes, L. Komzsik, J.G. Lewis, D.S. Scott and H.D. Simon, "Symmetric Generalized Eigenproblems in Structural Engineering," Minisymposium on Industrial Applications of Linear Algebra, Second SIAM Conference on Applied Linear Algebra, Raleigh, North Carolina, April 1985.

R.G. Grimes, J.G. Lewis and H.D. Simon, "Modern Eigenextraction Algorithms for Structural Dynamic Analyses," ICES '85 International Conference, Toronto, Ontario, August 1985.

R.G. Grimes, H. Krakauer, J.G. Lewis, H.D. Simon and S.H. Wei, "The Solution of Large Dense Generalized Eigenvalue Problems on the CRAY X-MP/24 with SSD," Second SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, Virginia, November 1985.

J.G. Lewis and H.D. Simon, "Platzman's Problem Revisited," Second SIAM Conference on Applied Linear Algebra, Raleigh, North Carolina, April 1985.

J.G. Lewis, "Eigenvalue Problems and Algorithms in Structural Engineering," IBM Europe Institute, Oberlech, Austria, July 1985.

J.G. Lewis, "Eigenvalue Problems and Supercomputers," BCS/NSF Supercomputer Summer Institute, Seattle, Washington, August 1985.

J.G. Lewis, "Modern Eigenextraction Algorithms for Structural Dynamic Analyses," ICES '85 International Conference, Toronto, Ontario, August 1985.

J.G. Lewis, B. Nour-Omid and H.D. Simon, "A Parallel Algorithm for the Symmetric Tridiagonal Eigenvalue Problem," Second SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, Virginia, November 1985.

J.G. Lewis and H.D. Simon, "The Impact of Hardware Gather/Scatter on Sparse Gaussian Elimination", 12th International Conference on Parallel Processing, St. Charles, Illinois, August 1986.

H.D. Simon, "Supercomputer Vectorization and Optimization," Annual Meeting of the American Mathematical Society, Anaheim, California, January 1985.

H.D. Simon, "Incomplete LU Preconditioners for Conjugate-Gradient-Type Iterative Methods," Eighth SPE Symposium on Reservoir Simulation, Dallas, Texas, February 1985.

H.D. Simon, R.G. Grimes, J.G. Lewis, L. Komzsik, and D. Scott "Shifted Block Lanczos Algorithm in MSC/NASTRAN," MSC/NASTRAN User's Conference, Los Angeles, California, March 1985.

H.D. Simon, "Supercomputers -Experience and the Future," 12th Annual ACM SIGUCCPS Computer Center Management Symposium, St. Louis, Missouri, March 1985.

H.D. Simon, "Principles of Vectorization," BCS/NSF Supercomputer Summer Institute, Seattle, Washington, August 1985.

H.D. Simon, "Memory and Memory Access on the Cray X-MP," BCS/NSF Supercomputer Summer Institute, Seattle, Washington, August 1985.

H.D. Simon, "Software and Algorithms for the Iterative Solution of Sparse Linear Systems on Supercomputers," BCS/NSF Supercomputer Summer Institute, Seattle, Washington, August 1985.

H.D. Simon, "Computational Kernels," First RIMSIG Meeting, Lawrence Livermore, California, October 1985.

H.D. Simon, "Approximate Inverses: A Family of Naturally Vectorizing Preconditioners," Second SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, Virginia, November 1985.

RECENT ABSTRACTS PREPARED FOR PRESENTATION AT PROFESSIONAL MEETINGS

The following abstracts are preliminary reports of work in progress.

R.G. Grimes, "Experiences in Solving Large Eigenvalue Problems on the Cray X-MP", Cray Users Group Meeting, Garmisch Partenkirchen, West Germany, September 1986.

R.G. Grimes, J.G. Lewis, H.D. Simon, "A Shifting Strategy for the Lanczos Algorithm", First International Congress on Computer Methods in Mechanical Engineering, Austin, TX, September 1986.

PROFESSIONAL PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

Four researchers from Boeing Computer Services, C. Cleveland Ashcraft, Roger G. Grimes, John G. Lewis, and Horst D. Simon performed most of the work during the first year of this contract. John G. Lewis acted as Project Manager. Task 5, which is concerned with the completion of the test matrix collection, is being carried out in collaboration with Dr. Iain S. Duff of AERE, Harwell, England.

RELATED SPARSE MATRIX ACTIVITIES AT BOEING COMPUTER SERVICES COMPANY

The mathematicians at Boeing Computer Services working on this project also are active in other projects which involve sparse matrix computations. This section briefly describes some of the most recent activities by those people. These projects are not funded by the AFOSR contract but they indicate the significant role that sparse matrix research plays at BCS.

Sparse Vector and Matrix Building Blocks for the CRAY X-MP. All four of the mathematicians on this project have been involved in developing, implementing and testing assembler language basic building blocks for sparse vector and matrix computations on the CRAY X-MP computer. These subprograms are a part of VectorPak. R.G. Grimes is the project lead for this Boeing commercial activity.

CRAY X-MP Optimization of SPARSPAK and COMPLEX version of SPARSPAK. J. G. Lewis and R. G. Grimes have modified SPARSPAK so that a version optimized for the CRAY X-MP and a COMPLEX version have been produced. Condition number estimator and stability monitoring have been added.

Out-of-Core Nested Dissection Code. J.G. Lewis continues the work on the solution of huge systems of linear equations by nested dissection algorithms. The linear systems have as many as one million equations and are derived from special finite element models with a very regular structure. This work is undertaken for a major commercial customer and represents a significant industrial production program.

Sparse Eigenanalysis for Structural Engineering. R.G. Grimes, J.G. Lewis, and H.D. Simon have implemented a block shifted and inverted Lanczos algorithm into the commercial structural engineering analysis package NASTRAN for the MacNeill-Schwendler corporation. This represents the state of the art for sparse matrix eigenanalysis. It has particular relevance to the present contract in that the sparse linear systems required are symmetric with indefinite coefficient matrix. Task 2 of this project will have direct impact on this application.

This project also included the incorporation of the same analysis techniques into the Boeing ATLAS structures program, and into the Boeing version of Georgia Tech's STRUDL program. These three packages, particularly NASTRAN, provide a rich source of useful test problems.

Iterative Methods and Preconditioners on Vector and Parallel Computers. C. Ashcraft, R. Grimes, and H.D. Simon are involved in the creation of a test bed

for iterative methods and preconditioners. The fully developed software will allow a user to investigate the efficiency of a particular preconditioner/iterative method combination for a particular application. C. Ashcraft has developed a variety of new preconditioning techniques, which extend his previous work on computational front techniques for regular grids. Computational front techniques can be implemented in a dataflow like manner on parallel machines. There has been a frequent cross germination of ideas between this internally funded research program and the current contract.

Analysis of Parallel Architectures. C. Ashcraft has recently implemented several industrial codes on hypercube computers. H. Simon is project lead for a Boeing project investigating current commercially available advanced architecture computers. R. Grimes is responsible for a benchmark activity involving these machines. C. Ashcraft and J. G. Lewis will participate in parallel architecture project, whose goals are to provide a focal point within Boeing for knowledge about parallel computing. J. G. Lewis will spend a sabbatical year in 1986/87 at MIT and Yale to study the potential applications of parallel architectures to scientific computing.

Software Tools for Supercomputers. H.D. Simon is Project Manager of this work funded by the Office of Advanced Scientific Computing at the NSF. The goal is to investigate tools for porting application programs to a parallel environment.

Large Dense Eigenanalysis. This project is part of the above mentioned NSF contract. H. Simon will extend the Lanczos work to solve dense generalized eigenvalue problems arising in quantum mechanical calculations. Particularly emphasis will be placed on an efficient out-of-core implementation of these algorithms.

Sparse Matrix Methods for Computational Fluid Dynamics. R. Grimes and H. Simon are involved in this joint project with the computational fluid dynamics research group at Boeing. The current approach of the CFD group requires the solution of linear systems with up to one million unknowns. A preconditioned iterative method, with the preconditioner based on a reduced system then still requires the exact solution of problems of about 30,000 equations using direct methods.

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